WHAT IS CLAIMED IS:

1. A method of preparing a crystal of CD40 ligand comprising the steps of:
   a) providing an aqueous solution comprising a fragment of CD40 ligand;
   b) providing a reservoir solution comprising a precipitating agent;
   c) mixing a volume of said aqueous solution with a volume of said reservoir solution thereby forming a mixed volume; and
   d) crystallizing at least a portion of said mixed volume.

2. The method of claim 1 wherein the aqueous solution of CD40 ligand provided in step a) has a concentration of CD40 ligand of about 1 to about 50 mg per ml.

3. The method of claim 2 wherein the aqueous solution has a concentration of CD40 ligand of about 5 mg per ml to about 15 mg per ml.

4. The method of claim 3 wherein the aqueous solution has a concentration of CD40 ligand of about 10 mg per ml.

5. The method of claim 1 wherein the precipitating agent is selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol.

6. The method of claim 1 wherein the concentration of the precipitating agent in the reservoir solution is about 1.0 M to about 1.5 M.

7. The method of claim 6 wherein the concentration of precipitating agent is about 1.2 M.

8. The method of claim 1 wherein the pH of the reservoir

solution is about 4 to about 10.

9. The method of claim 8 wherein the pH is about 7.5.

10. The method of claim 1 wherein step d) is by vapor diffusion crystallization, batch crystallization, liquid bridge crystallization or dialysis crystallization.

11. A crystal formed by a functional fragment of the extracellular domain of CD40 ligand having approximately the following cell constants: a+b=77.17 x 10^{-10} M (Å), c= 90.46 x 10^{-10} M (Å), $\alpha = \beta = 90°$, $\gamma = 120°$, and a space group of R3.

~~12. Deleted.~~

R1.126 12 13. A machine readable data storage medium comprising a data storage material encoded with machine readable data which, when read by an appropriate machine, is capable of displaying a three dimensional representation of a crystal of a molecule or molecular complex comprising a fragment of CD40L having a binding site comprising amino acids Lys143, Arg203, Arg207 and Tyr145.

R1.126 13 14. A crystal of CD40 ligand (116-261) according to claim 11, or a homolog thereof, wherein said crystal comprises a binding site, said binding site comprising amino acids Lys143, Arg203, Arg207 and Tyr145.

Rl.126 14 ~~15~~. A crystal according to claim 11 or a homolog thereof wherein said the crystal comprises Arg207 in close proximity to at least two hydrophobic residues.

R1.126 15. ~~16.~~ A crystal according to claim 14 wherein said crystal comprises at least 30 amino acids selected from the group consisting of: Ile127, Ser128, Glu129, Ala130, Ser131, Thr135, Ser136, Ala41, Lu142, Gly144, Tyr146, Cys178, Asn180, Ser185, Gln186, Ala187, Pro188, Ile190, Ala191, Ser192, Ser197, Pro198, Gly199, Arg200, Phe201, Glu202, Ile204, Ala209, Thr211, Pro217, Cys218, Gly219, Gln220, Glu230, Leu231, Gln232, Asn240, Val241, Thr242, Asp243, Ser245, Val247, Ser248, His249, Gly250, Thr251, Gly252 and Phe253.

R1.126 16. ~~17.~~ A crystal according to claim 16, wherein said binding site comprises amino acids Ile127, Ser128, Glu129, Ala130, Ser131, Thr135, Ser136, Ala141, Glu142, Lys143, Gly144, Tyr145, Tyr146, Cys178, Asn180, Ser185, Gln186, Ala187, Pro188, Ile190, Ala191, Ser192, Ser197, Pro198, Gly199, Arg200, Phe201, Glu202, Arg203, Ile204, Arg207, Ala209, Thr211, Pro217, Cys218, Gly219, Gln220, Glu230, Leu231, Gln232, Asn240, Val241, Thr242, Asp243, Ser245, Val247, Ser248, His249, Gly250, Thr251, Gly252 and Phe253.

R1.126 17. ~~18.~~ A method for determining at least a portion of a three dimensional structure of a molecular complex, said complex comprising at least a fragment of CD40 ligand, said method comprising the steps of:

a.) determining the structural coordinates of a crystal of the fragment of CD40 ligand;

b.) calculating phases from the structural coordinates;

c) calculating an electron density map from the phases obtained in step b);

d) determining the structure of at least a portion of the complex based upon said electron density map.

R1.126 18/~~19~~. The method of claim 18 wherein the structural coordinates used in step a) are (1) substantially the same as those described in Table 1 or (2) describe substantially the same crystal as the coordinates in Table 1.

R1.126 19/~~20~~. A method for evaluating the ability of a chemical entity to associate with CD40 ligand or CD40, a fragment of CD40 or CD40 ligand, or a complex comprising CD40 ligand, CD40, or homologs thereof, said method comprising the steps of:

a) employing computational or experimental means to perform a fitting operation between the chemical entity and said CD40 ligand or CD40, fragment or complex thereof, thereby obtaining data related to said association; and

b) analyzing the data obtained in step a) to determine the characteristics of the association between the chemical entity and said CD40 ligand or CD40, fragment or complex.

R1.126 20/~~21~~. A chemical entity having a molecular weight of less than 2000 daltons identified by the method of claim 20, wherein said chemical entity is capable of interfering with the in vivo or in vitro association between CD40 and CD40L.

R1.126 21/~~22~~. A chemical entity having a molecular weight of less than 2000 daltons identified by the method of claim 20, wherein said chemical entity is capable of associating

comprising amino acids Lys143, Arg203, Arg207 and Tyr145.

R1.126 22. A chemical entity having a molecular weight of less than 2000 daltons identified by the method of claim 20 wherein said chemical entity is capable of associating with CD40, and comprises a binding site comprising amino acids Lys143, Arg203, Arg207 and Tyr145.

amino acids Lys143, Arg203, Arg207 and Tyr145.

R1.126 23. ~~24~~. The chemical entity identified by the method of claim 22 or 23 wherein said CD40L binding site comprises at least 30 amino acids selected from the group consisting of: Ile127, Ser128, Glu129, Ala130, Ser131, Thr135, Ser136, Ala141, Glu142, Gly144, Tyr146, Cys178, Asn180, Ser185, Gln186, Ala187, Pro188, Ile190, Ala191, Ser192, Ser197, Pro198, Gly199, Arg200, Phe201, Glu202, Ile204, Ala209, Thr211, Pro217, Cys218, Gly219, Gln220, Glu230, Leu231, Gln232, Asn240, Val241, Thr242, Asp243, Ser245, Val247, Ser248, His249, Gly250, Thr251, Gly252 and Phe253.

R1.126 24. ~~25~~. The chemical entity of claim 23, wherein said entity is capable of associating with a binding site on CD40L, wherein said binding site comprises amino acids Ile127, Ser128, Glu129, Ala130, Ser131, Thr135, Ser136, Ala141, Glu142, Lys143, Gly144, Tyr145, Tyr146, Cys178, Asn180, Ser185, Gln186, Ala187, Pro188, Ile190, Ala191, Ser192, Ser197, Pro198, Gly199, Arg200, Phe201, Glu202, Arg203, Ile204, Arg207, Ala209, Thr211, Pro217, Cys218, Gly219, Gln220, Glu230, Leu231, Gln232, Asn240, Val241, Thr242, Asp243, Ser245, Val247, Ser248, His249, Gly250, Thr251, Gly252 and Phe253.

R1.126 25. ~~26~~. A heavy atom derivative of a crystallized form of CD40 ligand.

R1.126 26. ~~27~~. A heavy atom derivative of the crystal of claim 11.

R1.126 27. ~~28~~. The use of the structural coordinates of CD40 ligand, or portions thereof, to solve a crystal form of a mutant, homologue or co-complex of CD40 ligand or a fragment thereof by molecular replacement.

R1.126 ~~28.~~ 29. A method of computationally or experimentally evaluating a chemical entity to obtain information about its association with the binding site of CD40 ligand using a crystal of CD40 ligand or the structural coordinates thereof.

R1.126 ~~29.~~ 30. The method of claim 29 wherein the crystal has the structural coordinates described in Table 1.

R1.126 ~~36.~~ 31. The use of the structural coordinates of a crystal, wherein said crystal is substantially the same as the crystal of CD40 ligand described by the coordinates in Table 1.

R1.126 ~~31.~~ 32. The method of claim 29 wherein said crystal is a crystal according to claim 11.

R1.126 ~~32.~~ 33. The use of the structural coordinates of a crystal according to claim 31, to identify, characterize or design chemical entities having a desired association with a CD40 ligand, or fragment thereof.

R1.126 ~~33.~~ 34. The method of claim 33 further comprising the step of optimizing the binding characteristics of the chemical entity identified, characterized, or designed.

R1.126 ~~34.~~ 35. The method of claim 34 further comprising the step of determining the orientation of ligands in a binding site of CD40 ligand.

R1.126 35. ~~36.~~ A chemical entity having a molecular weight of less than 2000 daltons identified or designed according to claim 33.

R1.126 36. ~~37.~~ The use of a CD40 ligand crystal to determine binding interactions between a chemical entity and CD40 ligand.

AMENDED SHEET

R1.126 37. ~~38~~. The use according to claim 37 wherein said CD40 ligand crystal is the crystal of claim 11.

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